

Supporting Information

Effect of Ethylene-, Diethylene-, Triethylene Glycols and Glycerol on Physico-Chemical Properties and Phase Behavior of Benzyltrimethyl and Benzyltributylammonium chloride based Deep Eutectic Solvents at 283.15 to 343.15 K

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Calculation of molecular weight:

$$M_{DES} = x_{Salt}M_{Salt} + x_{HBD}M_{HBD}$$

Table S1: Glass transition temperature data for different mole ratios of HBA to HBDs for BTMGLY.

Mole ratio of HBA:HBD	Glass transition temperature (T_g /K)
2:1	192.8
1:1	197.6
1:2	195.9
1:3	191.3
1:4	192.4

Table S2: IR spectra regions of synthesized DES.

Wavenumber (cm ⁻¹)	Allotment of Regions
3400-3300	OH stretching vibrations
3100-3000	Aromatic stretching vibrations
2900-2850	Aliphatic stretching vibrations
1650 and 1470-1450	C=C and C-C ring stretching
1410-1400	C-OH bending vibrations
1120-1050	C-O and C-O-C stretching vibration
840-800	OH wagging vibration
750-700	Aromatic CH wagging vibration

Table S3: Calculated values of thermal expansivity, α (Eq. 4) for synthesized DES at temperature, T= (283.15 to 343.15) K and pressure, $p = 0.1\text{MPa}$ ^a

$10^4 \times \alpha / \text{K}^{-1}$								
<i>T/K</i>	BTMEG	BTMDEG	BTMTEG	BTMGly	BTBEG	BTBDEG	BTBTEG	BTBGly
283.15	5.44	5.57	5.94	4.97	6.03	5.81	6.07	5.64
288.15	5.45	5.59	5.96	4.99	6.05	5.83	6.09	5.65
293.15	5.47	5.60	5.98	5.00	6.06	5.85	6.11	5.67
298.15	5.48	5.62	5.99	5.01	6.08	5.87	6.13	5.68
303.15	5.50	5.63	6.01	5.02	6.10	5.88	6.15	5.70
308.15	5.51	5.65	6.03	5.04	6.12	5.90	6.17	5.72
313.15	5.53	5.66	6.05	5.05	6.14	5.92	6.19	5.73
318.15	5.54	5.68	6.07	5.06	6.16	5.94	6.21	5.75
323.15	5.56	5.70	6.08	5.07	6.18	5.95	6.22	5.77
328.15	5.57	5.71	6.10	5.09	6.20	5.97	6.24	5.78
333.15	5.59	5.73	6.12	5.10	6.22	5.99	6.26	5.80
338.15	5.60	5.75	6.14	5.11	6.23	6.01	6.28	5.82
343.15	5.62	5.76	6.16	5.13	6.25	6.02	6.30	5.83

^a Standard uncertainties u are $u(\alpha) = 0.02 \text{ kK}^{-1}$, $u(T) = 0.01 \text{ K}$ and $u(p) 10 \text{ kPa}$.

Table S4: Calculated values of intermolecular free length, L_f (from Eq.7) for synthesized DES at temperature, T= (293.15 to 323.15) K and pressure, $p = 0.1\text{MPa}$ ^a

$L_f/\text{\AA}$								
T/K	BTMEG	BTMDEG	BTMTEG	BTMGly	BTBEG	BTBDEG	BTBTEG	BTBGly
293.15	0.321	0.334	0.334	0.291	0.357	0.359	0.356	0.321
298.15	0.328	0.340	0.341	0.297	0.365	0.363	0.364	0.330
303.15	0.334	0.347	0.348	0.302	0.373	0.367	0.372	0.338
313.15	0.345	0.359	0.361	0.312	0.388	0.370	0.387	0.352
323.15	0.356	0.371	0.374	0.322	0.402	0.374	0.401	0.365

^a Standard uncertainties u are $u(T) = 0.01\text{ K}$ and $u(p) 10\text{ kPa}$.

Table S5: Calculated values of isentropic compressibility, β_s (Eq. 8) for synthesized DES at temperature, T= (283.15 to 343.15) K and pressure, $p = 0.1\text{MPa}$ ^a

$\beta_s / \text{TPa}^{-1}$								
<i>T</i> /K	BTMEG	BTMDEG	BTMTEG	BTMGly	BTBEG	BTBDEG	BTBTEG	BTBGly
283.15	261.3	281.0	281.1	211.5	317.8	322.6	317.2	247.0
288.15	265.8	286.1	286.9	216.7	325.8	330.3	324.9	258.9
293.15	270.3	291.3	292.6	221.3	333.5	337.7	332.4	269.2
298.15	274.8	296.4	298.6	225.4	341.1	344.9	339.9	278.3
303.15	279.5	301.6	304.5	229.3	348.8	352.1	347.4	286.4
308.15	284.2	306.9	310.6	233.1	356.5	359.2	354.9	293.9
313.15	289.0	312.3	316.8	236.8	364.3	366.5	362.6	300.9
318.15	293.9	317.7	323.0	240.6	372.3	373.9	370.4	307.7
323.15	298.9	323.3	329.4	244.4	380.4	381.3	378.3	314.2
328.15	304.0	328.9	335.9	248.3	388.7	389.0	386.4	320.7
333.15	309.2	334.7	342.6	252.2	397.1	396.7	394.6	327.3
338.15	314.5	340.5	349.4	256.2	405.7	404.6	403.0	333.8
343.15	319.8	346.3	356.3	260.1	414.2	412.4	411.3	340.3

^a Standard uncertainties u are $u(\beta_s) = 0.05 \text{ TPa}^{-1}$, $u(T) = 0.01 \text{ K}$ and $u(p) = 10 \text{ kPa}$.

Table S6: Fitting parameters, η_∞ and E_η of Arrhenius equation and regression values, R^2 for viscosity values of synthesized DES

	BTMEG	BTMDEG	BTMTEG	BTMGLY	BTBEG	BTBDEG	BTBTEG	BTBGLY
$\eta_\infty \times 10^6 /$ mPa·s	124.67	11.09	3.82	0.16	2.52	2.70	6.73	0.07
$E_\eta /$ kJ·mol ⁻¹	460.3	574.9	650.4	800.0	667.1	668.2	627.3	867.4
R^2	0.994	0.995	0.998	0.995	0.998	0.998	0.998	0.998

Table S7: Experimental weight percentage composition (wt %) data for studied pseudo ternary systems containing [BTMA]Cl based DES, K₃PO₄ and water at temperature of 298.15 K and pressure of 0.1MPa ^a

K ₃ PO ₄	[BTMA] Cl	K ₃ PO ₄	BTM EG	K ₃ PO ₄	BTM DEG	K ₃ PO ₄	BTM TEG	K ₃ PO ₄	BTM GLY
4.54	38.67	10.46	54.88	9.15	49.27	4.68	52.66	17.07	49.57
5.73	35.49	11.62	52.66	10.66	45.23	5.67	48.97	17.57	47.21
6.91	33.17	12.18	50.56	11.76	43.22	8.00	44.41	17.99	45.56
8.79	29.43	13.86	45.23	12.45	41.79	10.55	38.94	18.47	43.91
10.48	26.60	15.42	40.98	13.19	40.62	12.55	34.73	19.21	40.27
11.81	24.34	17.06	35.87	13.65	39.45	14.06	31.54	20.10	37.82
13.50	21.70	18.55	32.34	14.45	37.44	16.14	28.32	20.78	35.15
14.84	19.54	19.68	29.15	15.16	36.15	17.84	25.63	21.68	31.91
16.02	17.94	20.66	26.94	15.81	34.81	19.40	23.05	22.25	30.27
17.20	16.28	21.35	24.74	16.57	33.37	20.60	20.85	22.82	27.99
18.30	14.97	22.18	23.06	17.66	31.49	21.89	19.19	23.42	25.96
19.13	13.78	23.06	20.69	18.41	30.12	22.80	17.63	23.96	24.38
20.00	12.81	23.78	19.11	19.14	28.78	23.68	16.43	24.61	22.58
20.71	11.98	24.56	17.57	19.81	27.41	24.97	14.78	25.19	21.10
21.26	11.18	25.30	15.92	20.42	26.29	25.85	13.34	25.64	19.65
22.30	10.08	26.22	14.21	21.43	24.27	26.74	12.24	26.33	18.43
23.28	8.94	26.94	12.89	22.35	22.71	27.72	10.86	26.95	17.04
24.35	7.95	27.58	11.19	23.08	21.22	28.73	9.62	27.34	15.77
25.42	6.94	28.64	9.61	24.04	19.15	29.57	8.51	28.06	14.41
25.97	6.43	29.19	8.71	24.88	17.64	30.20	7.75	28.53	13.22
26.45	5.99	30.35	7.85	25.77	16.26			29.16	11.97
27.08	5.51	31.47	7.18	26.57	14.79			29.74	10.99
27.64	5.06	32.69	6.45	27.29	13.57			30.48	10.08
28.13	4.68	33.81	5.91	27.95	12.30			30.74	9.37
		35.09	5.33	28.61	11.20				
				29.35	10.03				
				30.00	9.04				
				30.86	7.99				
				31.83	6.86				

^a Standard uncertainties u are $u(w) = 0.0005$, $u(T) = 0.01$ K and $u(p) = 10$ kPa.

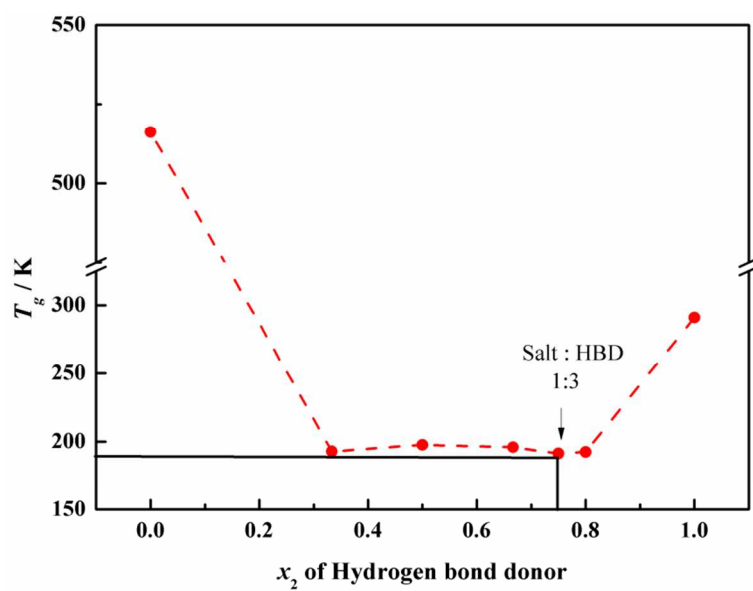


Figure S1. Phase diagram representing variation of glass transition temperature, T_g as a function of mole fraction (x_2) of hydrogen bond donor for BTMGLY.

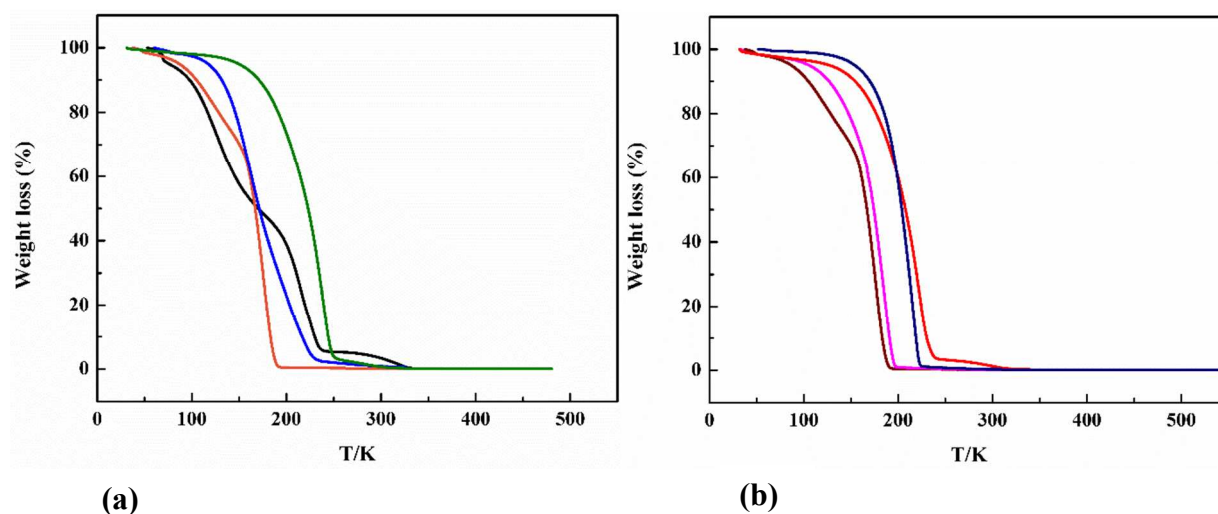


Figure S2: Thermo gravimetric analysis graphs of synthesized DES samples. Graphs represent the percentage weight loss with variation in temperature, T. (a) ■ BTMEG; ▲ BTMDEG; ● BTMTEG; ◆ BTMGly (b) ▼ BTBEG; ● BTBDEG; ★ BTBTeg; ► BTBGly.

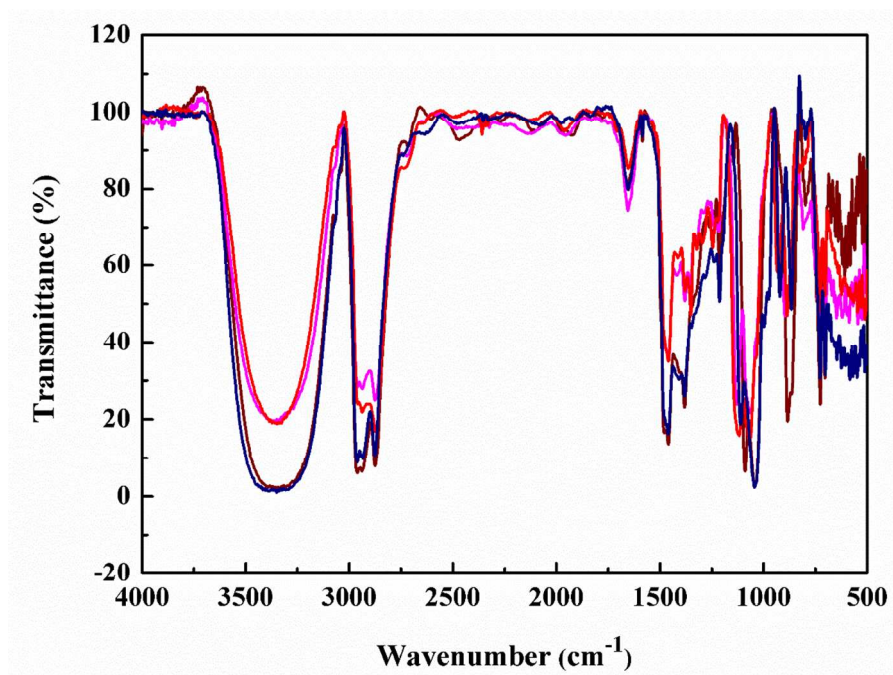


Figure S3: FT-IR spectra for the synthesized DES based on [BTBA]Cl. Wine, Magenta, Red and Navy colored lines represent BTBEG, BTBDEG, BTBTEG and BTBGLY respectively.